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14. ABSTRACT

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a. REPORT	b. ABSTRACT	c. THIS PAGE			Leilani Richardson
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62 Separate items are enclosed

~~DDRE0000X~~
2303M2C8

MEMORANDUM FOR PR (In-House Publication)

FROM: PROI (TI) (STINFO) 18 May 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-TP-2000-117**
Perkins, Dr. Leslie, "Computational Chemistry and Materials Science CTA"

High Performance Computing Mod. Office **(Statement A)**
(no location given, 27 Mar 00) **(Submission Deadline: N/A)**

1. This request has been reviewed by the Foreign Disclosure Office for: a.) appropriateness of distribution statement, b.) military/national critical technology, c.) export controls or distribution restrictions, d.) appropriateness for release to a foreign nation, and e.) technical sensitivity and/or economic sensitivity.
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Comments:_____

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Comments:_____

APPROVED/APPROVED AS AMENDED/DISAPPROVED

_____

LESLIE. S. PERKINS, Ph.D (Date)
Staff Scientist
Propulsion Directorate

PR2000 CHSSI Review

Computational Chemistry and Materials Science CTA

Dr. Leslie S. Perkins

CTA Leader

U.S. Air Force Research Laboratory

Propulsion Directorate

Edwards AFB, CA

CCM Concerns within DoD

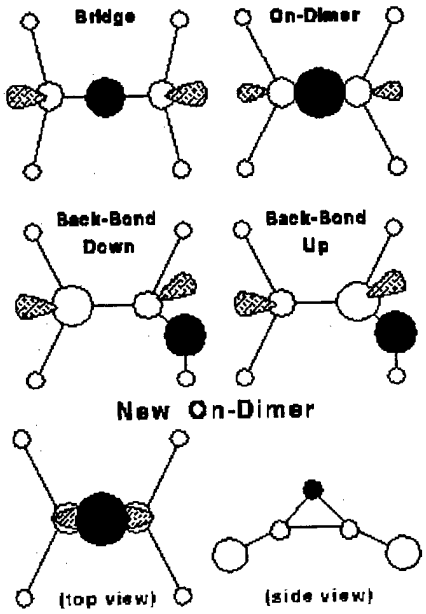
- Conductive and insulative materials for communications systems and sensors
- Aging and Surveillance of DoD stockpiles
- Contaminant decomposition within a known environment
- Energetic fuels and oxidizers for propulsion in critical military systems
- Low-observable coatings to protect the warfighter

Project Summary

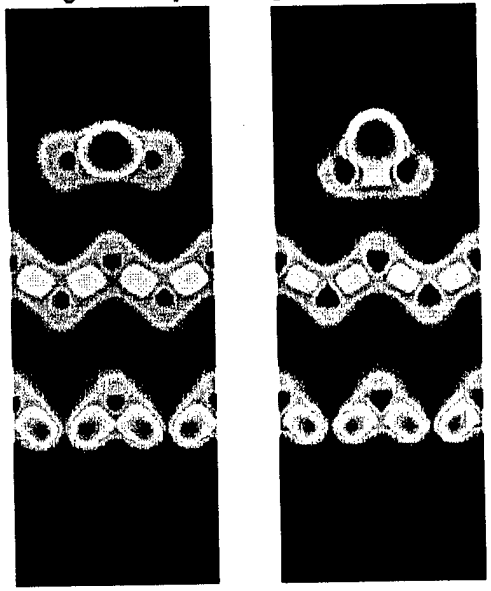
Project	*Scalability Range*	*Platforms*	*Deliverables*
CCM-1 : Car-Parrinello Methods for Solids	*23% - 70%*	*Origin 2000* *IBM SP*	*ACRES* *DoDPW*
CCM-2: Quantum Chemistry	*60% - 80%*	*IBM SP* *Cray T3E*	*GAMESS* *SAPT*
CCM-3: Tight Binding Molecular Dynamics	*62% - 97%*	*Origin 2000* *IBM SP*	*TBLibrary* *Static* *TBMD*
CCM-4: Classical Molecular Dynamics	*44% - 80%*	*Origin 2000* *Cray T3E*	*FMD* *PIMD/CMD*

CCM-1: Car-Parrinello Methods for Solids

- *Synopsis*
  - ***Objective***: Produce density functional codes (Car-Parrinello) to be used in DoD materials research
  - ***Partners:*** Harvard, NRL
  - ***Development Paradigm***:
    - DoDPW: FORTRAN90, C, MPI
    - ACRES: FORTRAN90, C, HPF



- Charge Density of Bridge and On-Dimer



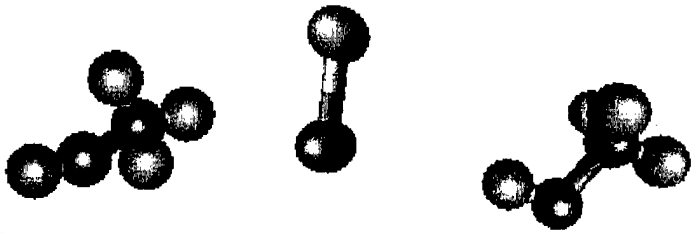
- *Performance*
  - ***Beta*** *Testing Complete*
  - *Scalability: (32 P.E.)*

	SP	*O2K*
DoDPW	*52*	*31*
ACRES	*47*	*25*

- *Management*
  - *Leveraging: NRL, ONR (Harvard)*
  - *Transition Approach: Code supported by NRL*
  - *Funding $1,672K (FY96-00)*

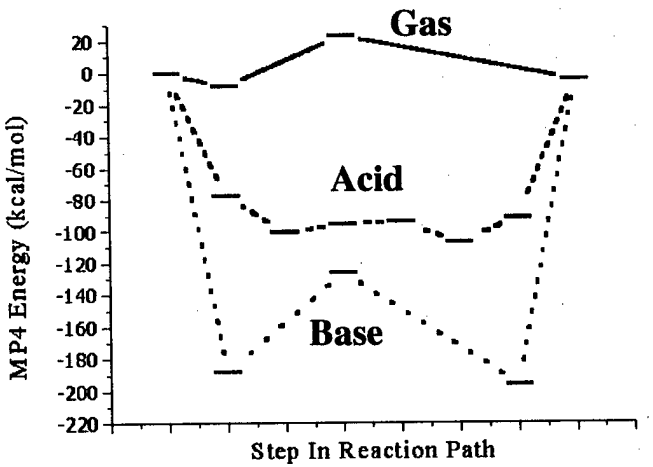
CCM-2: Quantum Chemistry

- *Synopsis*
  - ***Objective***: Produce ab initio chemistry codes to investigate new chemical species
  - ***Partners***: *AFRL/ML, U. of Delaware, Iowa State U.*
  - ***Development Paradigm***: FORTRAN77, MPI



Base Catalysis - POSS synthesis

Reaction Pathways – Formation of POSS



- *Performance*
  - ***Beta*** *Testing Complete*
  - *Scalability: 57% (SP)*
    50% (O2K)
  - *Operating Platforms: SP, O2K*

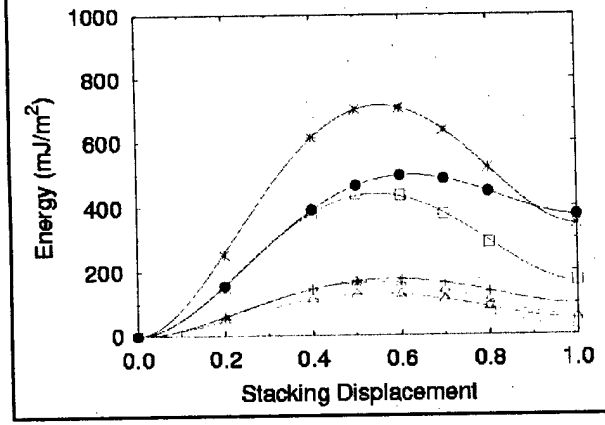
- *Management*
  - *Leveraging: DoE, NSF*
  - *Transition Approach: Used by 1,000+ users world-wide*
  - *Funding $1,593K (FY96-00)*

CCM-3: Tight Binding Molecular Dynamics

- *Synopsis*
  - ***Objective***: Develop a general purpose tight-binding MD code and associated libraries
  - ***Partners***: *Ohio State University, George Mason University* — To be consistent w/ others
  - ***Development Paradigm***: FORTRAN77, MPI

First Principles Calculation of Mechanical Properties: Stacking Fault Energies and Ductility Criterion

D. A. Papaconstantopoulos and M. J. Mehl
Center for Computational Materials Science
Naval Research Laboratory
Washington DC



		γ_s	γ_{us}	D
○	Ir	2590	902	0.87
*	Rh	2460	714	1.04
•	Pt	2510	497	1.53
□	Pd	1570	439	1.08
+	Al	870	176	1.50
△	Pb	888	166	1.59
×	Cu	1730	162	3.24
△	Au	1480	129	3.48
□	Ag	1140	108	3.20

- *Performance*
  - ***Beta*** *Testing Complete*
  - *Scalability: (16 P.E.)*

	SP	O2K
Fitting	-	**40**
Static	**50**	**95**
TBMD	**62**	**97**

- *Management*
  - *Leveraging: NRL*
  - *Transition Approach: Supported by NRL*
  - *Funding $1,954K (FY96-00)*

CCM-4: Classical Molecular Dynamics

- *Synopsis*
  - ***Objective***: Develop a molecular dynamics package that can realistically simulate large molecular systems for long time scales
  - ***Partners***: *AFRL, ARL, Iowa State U., U. of Utah, U. of Michigan, U. of Houston, Cornell U.*
  - ***Development Paradigm***: FORTRAN77, MPI

- *Performance*
  - ***Beta*** *Testing Complete*
  - *Scalability:*

	T3E	SP	O2K
FMD	40	40	44
CMD	-	85	80

- *Management*
  - *Leveraging: AFRL, AFOSR*
  - *Transition Approach: Supported by AFRL*
  - *Funding $1,793K (FY96-00)*

Applications of CHSSI Technology

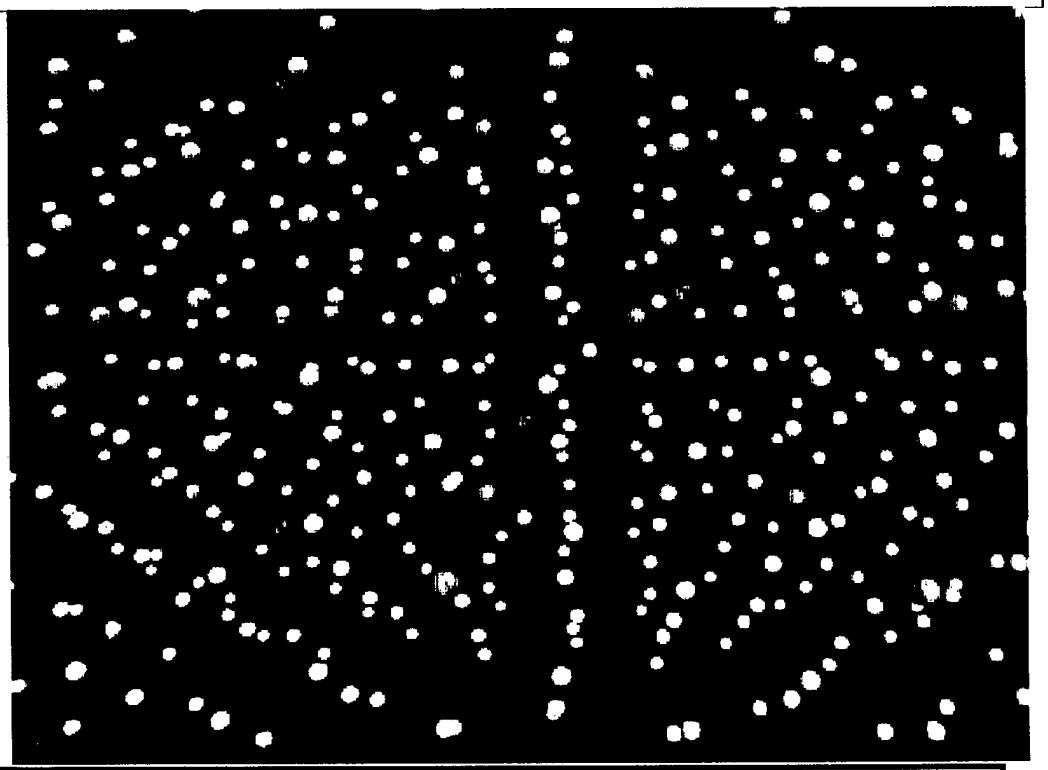
- *Problem*
  - ***Objective***: Is there global recombination of boron atoms in a solid hydrogen matrix if a single recombination is initiated?
  - ***Technology Used:*** *CMD (CCM-4)*
  - ***Technical Team***: U. of Utah, AFRL/PR

Hydrogen ○

Non-reacting Boron atom ○

Reacting Boron atom ○

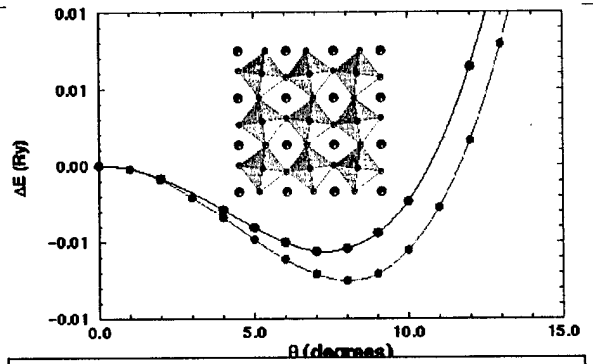
are these supposed to be different?



- *Impact...*
  - ***of Code Application:*** The thermal conductivity of the hydrogen matrix is sufficient to prevent global recombination of boron atoms in solid hydrogen
  - ***of CHSSI***: This calculation would be take over ~~1~~ one year, possibly two, to complete. The parallel CMD performs the calculations in ~~5~~ five weeks on 64 nodes of an IBM SP.

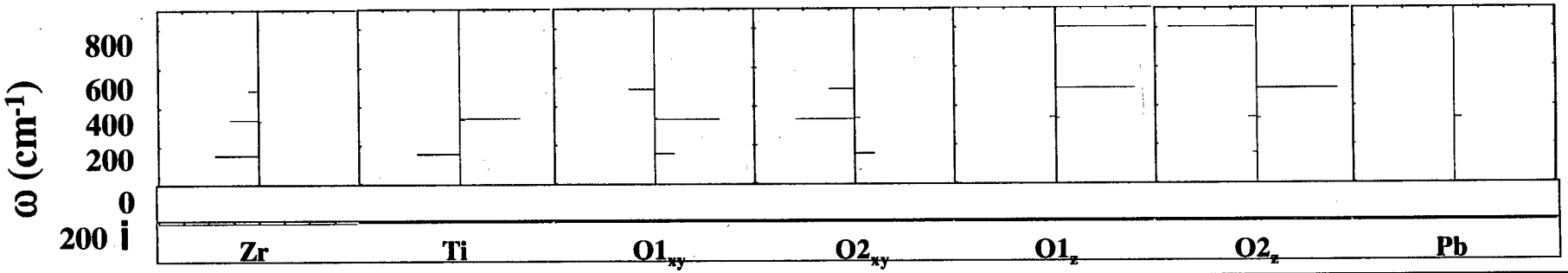
Applications of CHSSI Technology

- *Problem*
  - ***Objective***: Determine if Pb can be removed from PZT **[Pb(Zr,Ti)O_3]** a Navy Sonar Material, and maintain its effectiveness
  - ***Technology Used:*** DoDPW, NRL-LAPW
  - ***Technical Team***: NRL, ONR



Rotational Instability in Ferroelectric PZT 50-50 supercell.

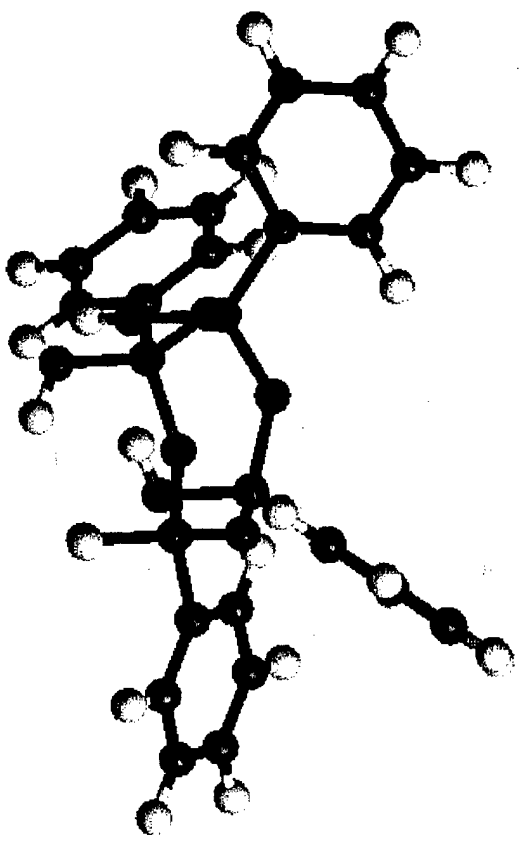
Phonon displacement patterns and frequencies in PZT 50-50 supercell



- *Impact...*
  - ***of Code Application:*** ONR and NRL are gaining a crucial understanding of how the Pb effects the sonar material
  - ***of CHSSI***: The code accurately describes the material and researchers will be able to suggest effective substitutes within a short time

Applications of CHSSI Technology

- *Problem*
  - ***Objective***: Identify important factors in the synthesis of polyhedral oligomeric silsesquioxanes (POSS) to modify the existing lengthy synthesis process
  - ***Technology Used:*** GAMESS (CCM-2)
  - ***Technical Team***: AFRL, Iowa State U., ASC MSRC PET



- *Impact...*
  - ***of Code Application:*** The effects of solvents led to a new process for the formulation of POSS. of different catalysts and solvents have been found to be crucial in the quick formulation of POSS.
  - ***of CHSSI***: The calculation to determine the structure and associated energies lasted approximately ~~1~~ one week. The serial version would require over ONE YEAR of dedicated time.